DEGAS 2 UPDATE:

EIRENE BENCHMARK

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INTRODUCTION

- Begin UEDGE coupling process by benchmarking against EIRENE.
- Slab "single-null" geometry,
- UEDGE plasma.
- Find:
  - Codes agree to within 5% when using the same physics,
  - Remaining 5% due to differences in numerical details.
  - Run time is about the same for both.
  - Also have MPI version of code running on SGI and T3E.
  - Recombination and toroidal geometry examined next.

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COMPARISON OF PHYSICS COMPONENTS

- Use DEGAS 2 standalone codes,
- EIRENE: hardwire “input” values and write out data.
- Checked: (see plots)
  1. Distribution of launch points,
  2. Energy distribution for reflection off Mo,
  3. Angular distribution for reflection,
  4. Angular distribution for off-normal incidence,
  5. Velocity distribution of desorbed D_2.

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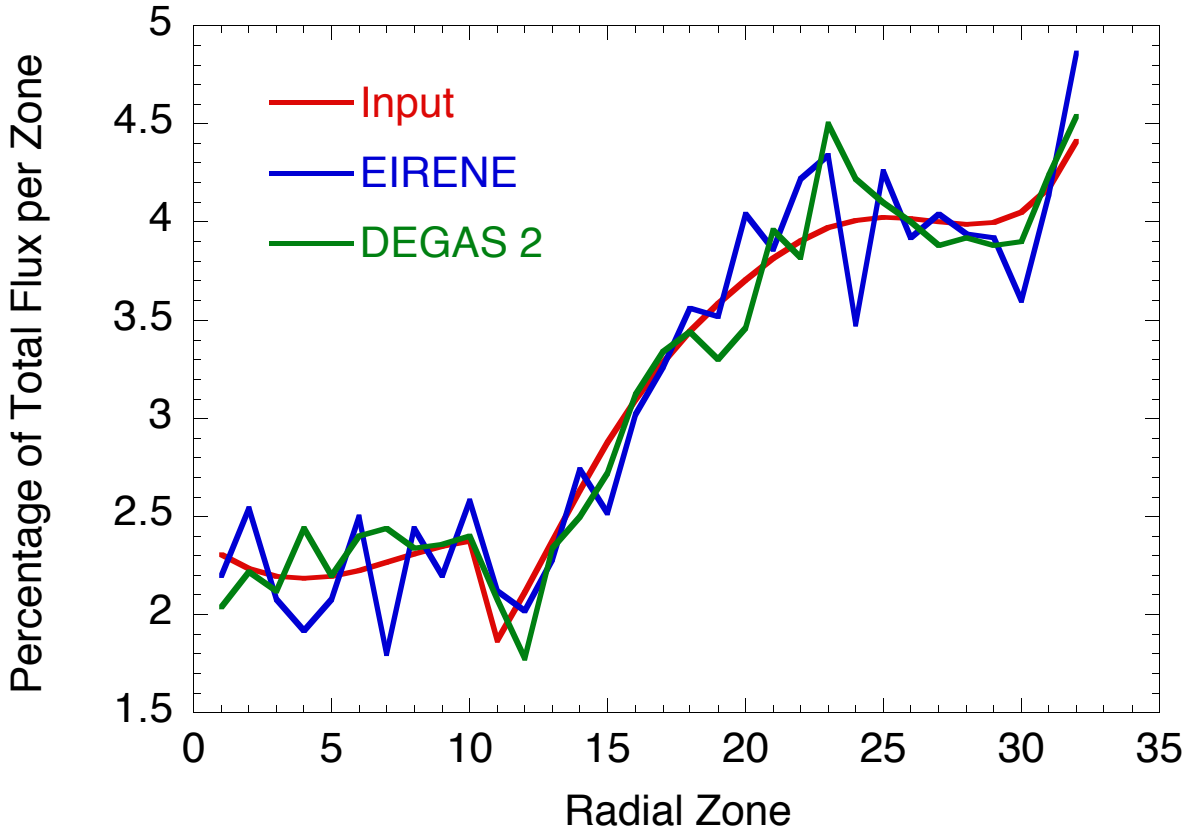
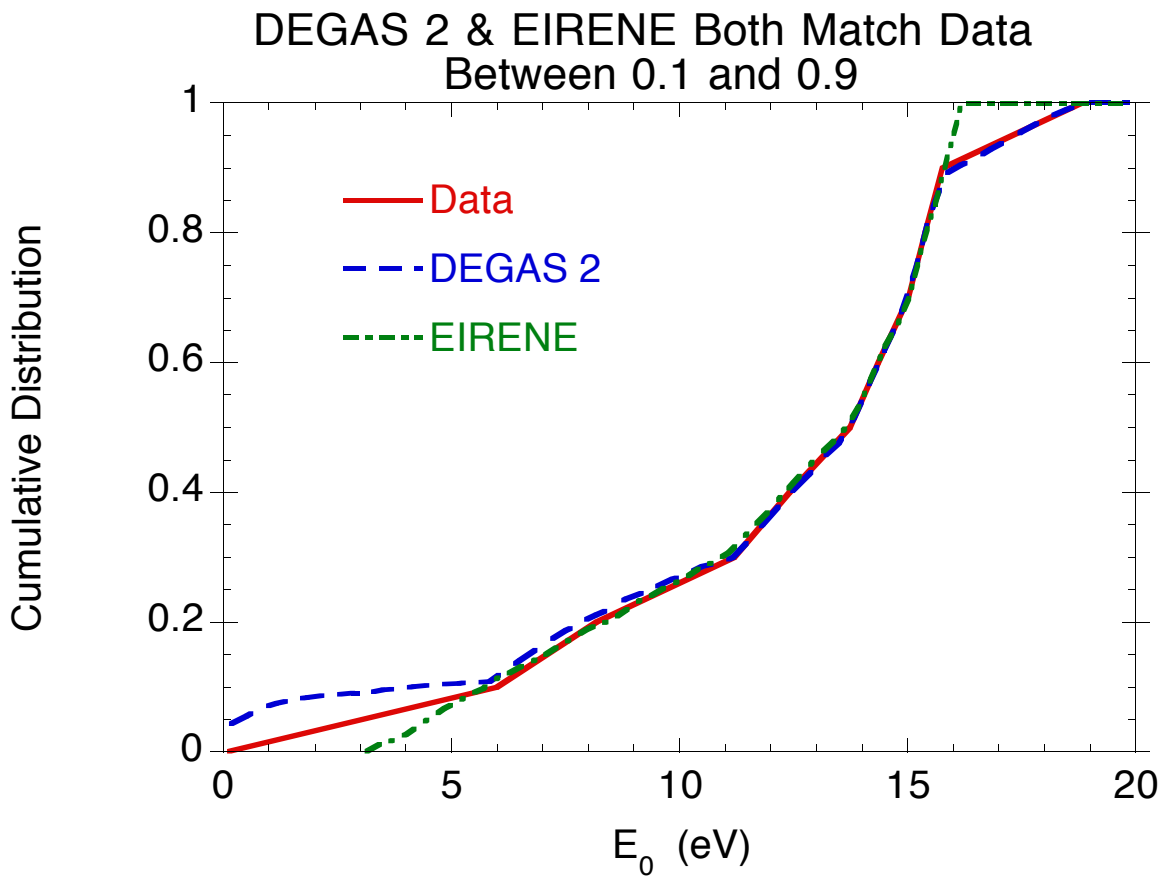
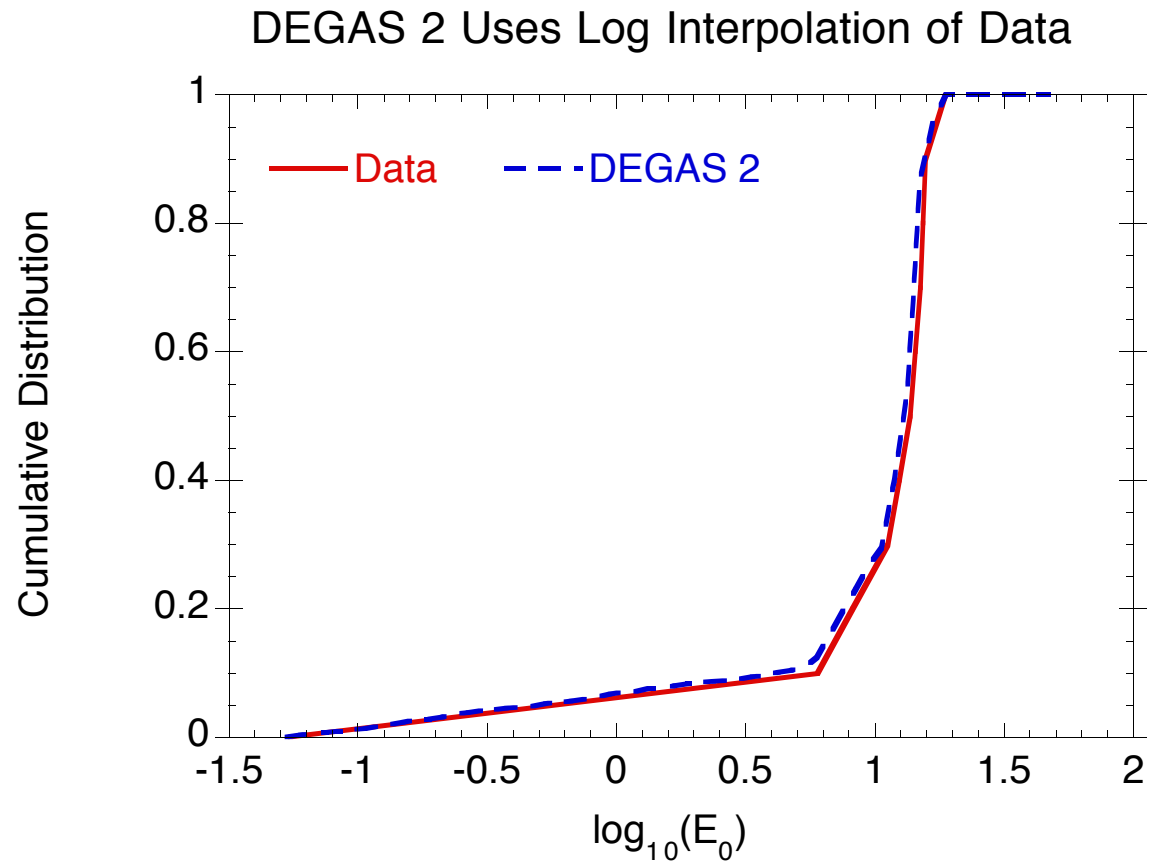
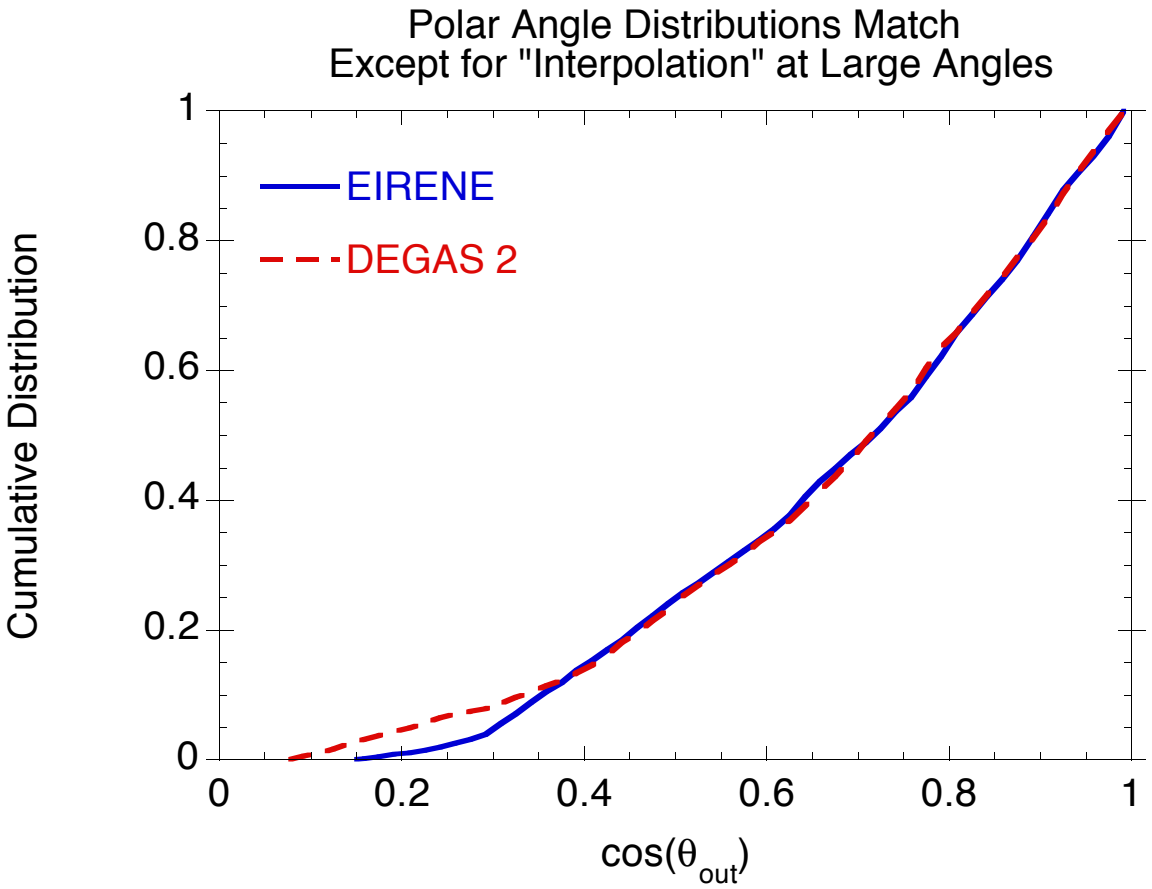
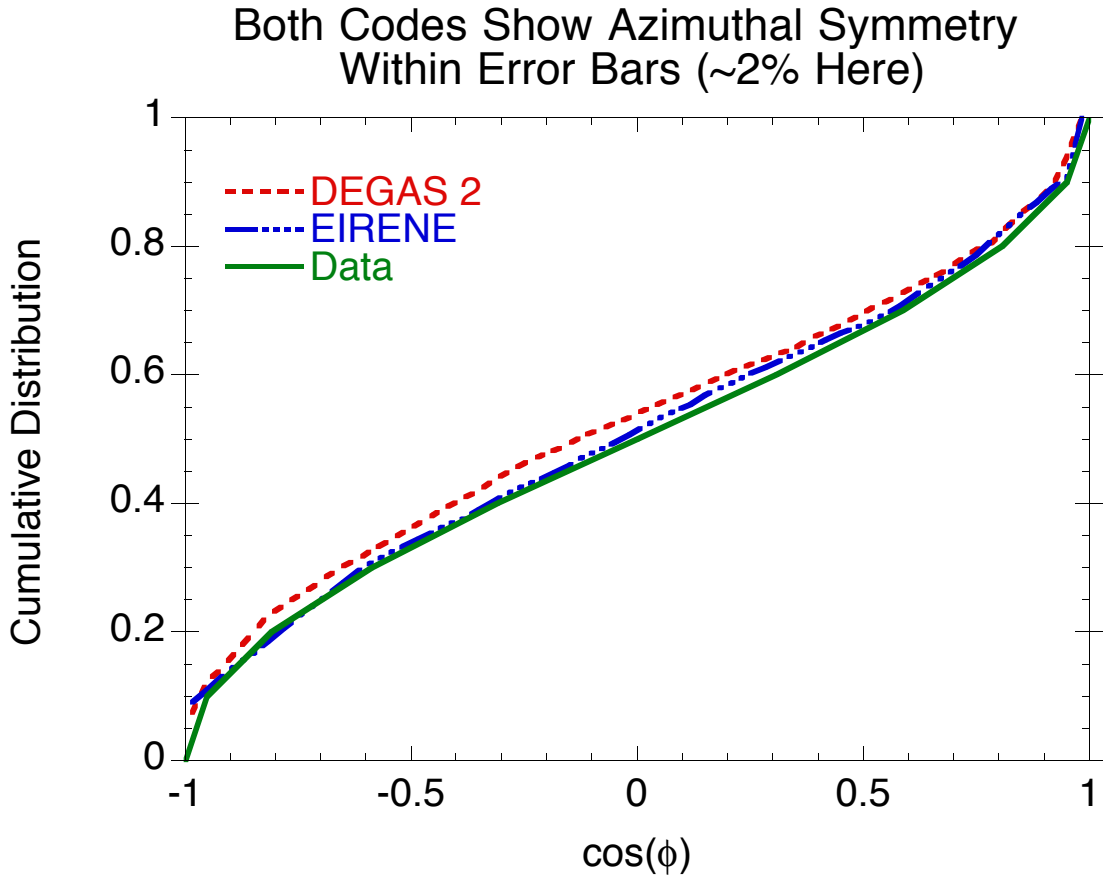
Both Codes Correctly Sample the Prescribed Flux Distribution



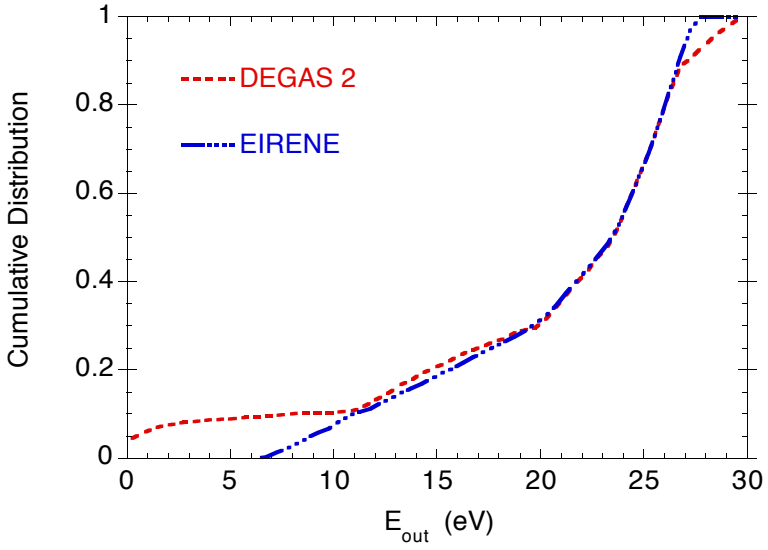

DEGAS 2 & EIRENE Both Match Data
Between 0.1 and 0.9
Cumulative Distribution
Data
DEGAS 2
EIRENE
0
0.2
0.4
0.6
0.8
1
0
5
10
15
20
E0 (eV)

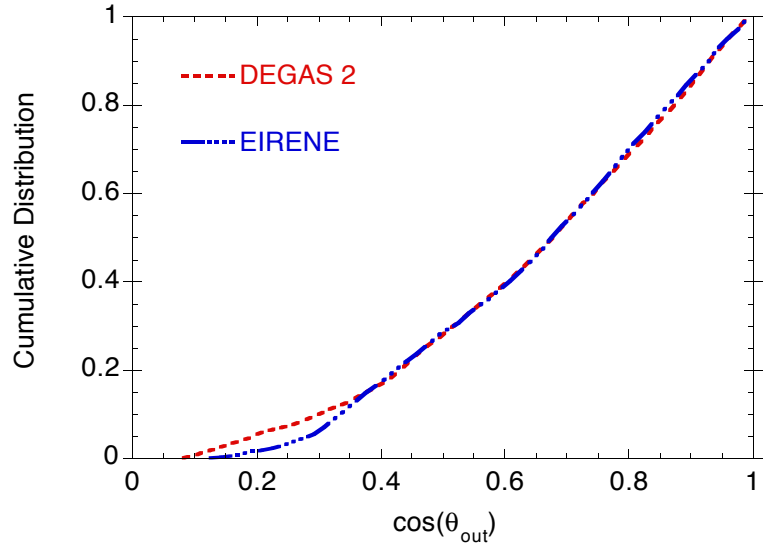

DEGAS 2 Uses Log Interpolation of Data
Cumulative Distribution
Data
DEGAS 2
0
0.2
0.4
0.6
0.8
1
-1.5
-1
-0.5
0
0.5
1
1.5
2
log10(E0)


Polar Angle Distributions Match
Except for "Interpolation" at Large Angles
EIRENE
DEGAS 2
Cumulative Distribution
cos(θout)
0
0.2
0.4
0.6
0.8
1

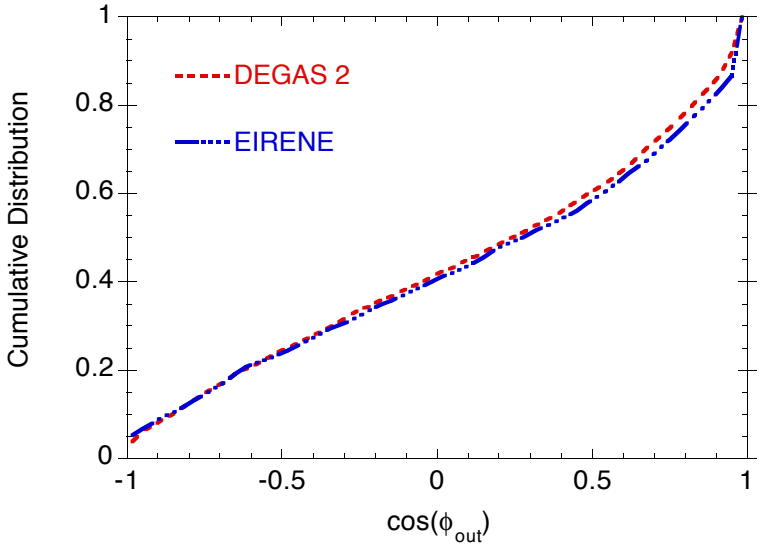

Both Codes Show Azimuthal Symmetry
Within Error Bars (~2% Here)
DEGAS 2
EIRENE
Data
Cumulative Distribution
cos(ϕ)
-1
-0.5
0
0.5
1

The Codes Agree Except
Outside the Bounds of the Data





For This Case: E_{in} = 30 eV, θ_{in} = 40°



RUNS WITH PARTIAL PHYSICS

1. No physics,
   - 3 eV D atom, launched with cosine distribution,
   - Bounces off mirrors until it exits.
   - At 200,000 flights, codes agree to within error bars (10 – 20%).
2. Add D ionization and charge exchange,
   - Agree to within error: 7%,
   - Differences in rate interpolations responsible for a few %.
3. Ion plate source from Mo, turn off CX,
   - Results differed by 20% near target,
   - Due to sensitivity of density to low energy reflections,
   - Modify DEGAS 2 data to mimic EIRENE extrapolation:
   - Some interpolation differences persist.
4. Add CX,
   - Get statistical agreement to within 5% error bars.

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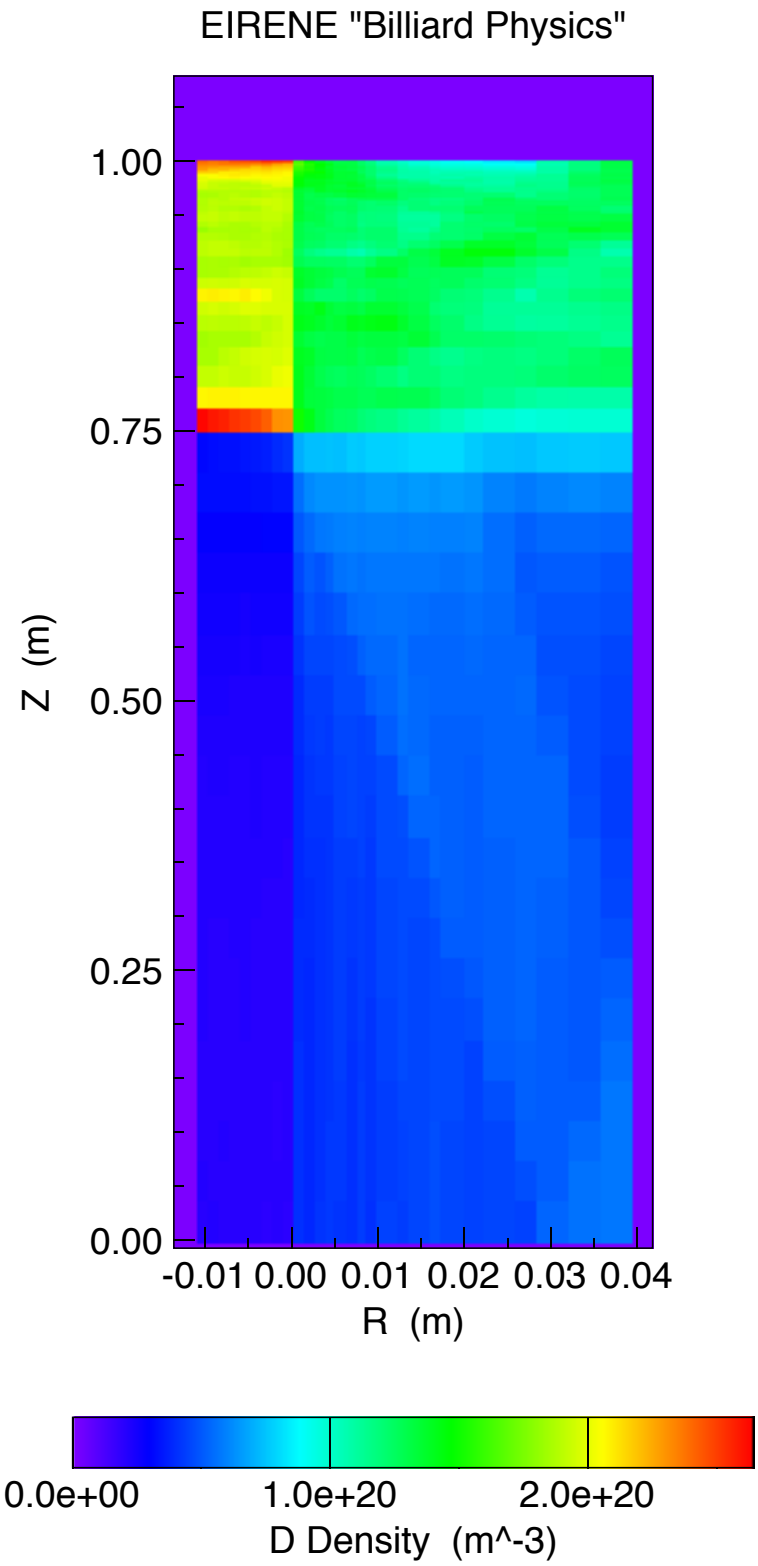
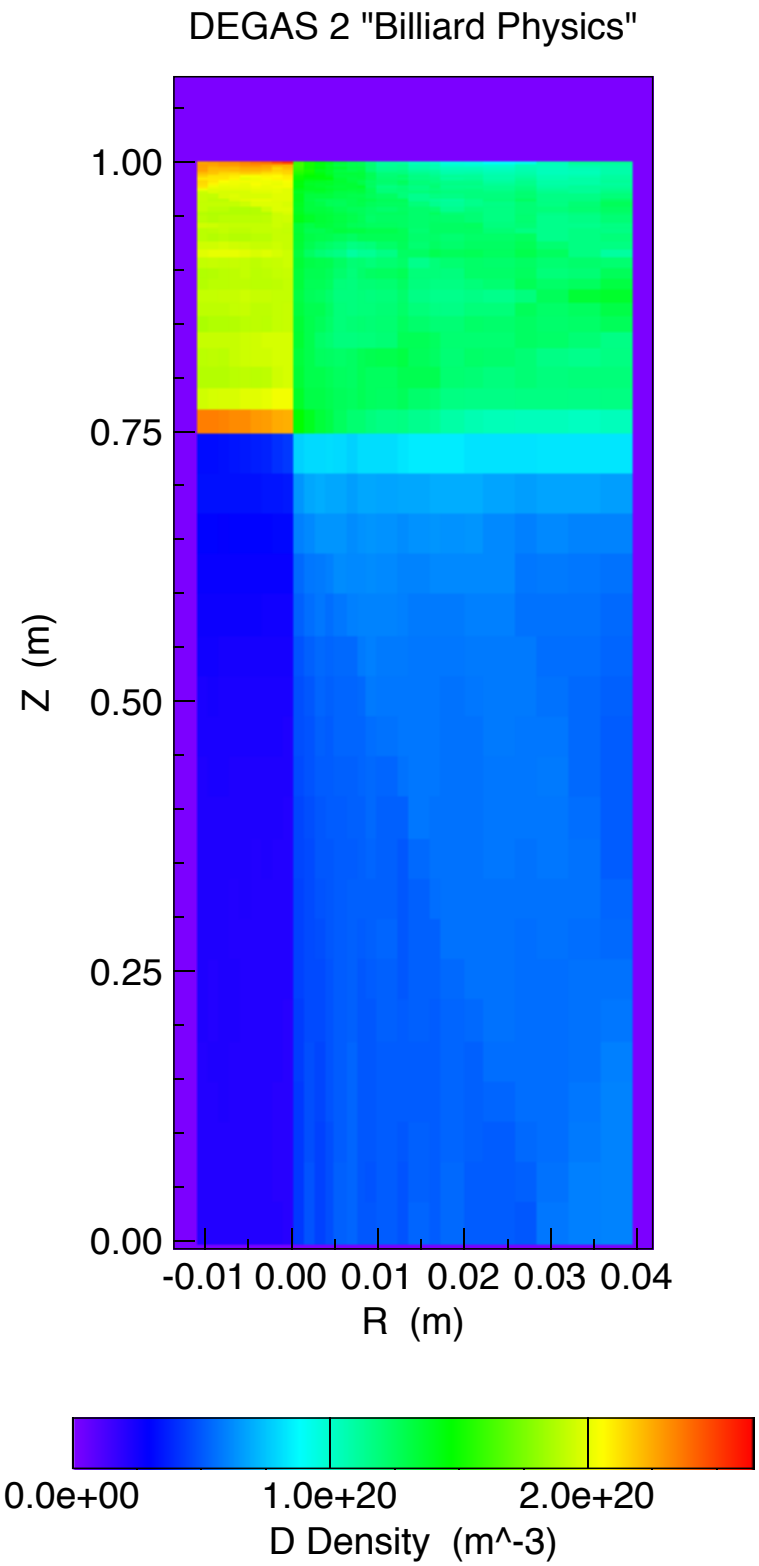
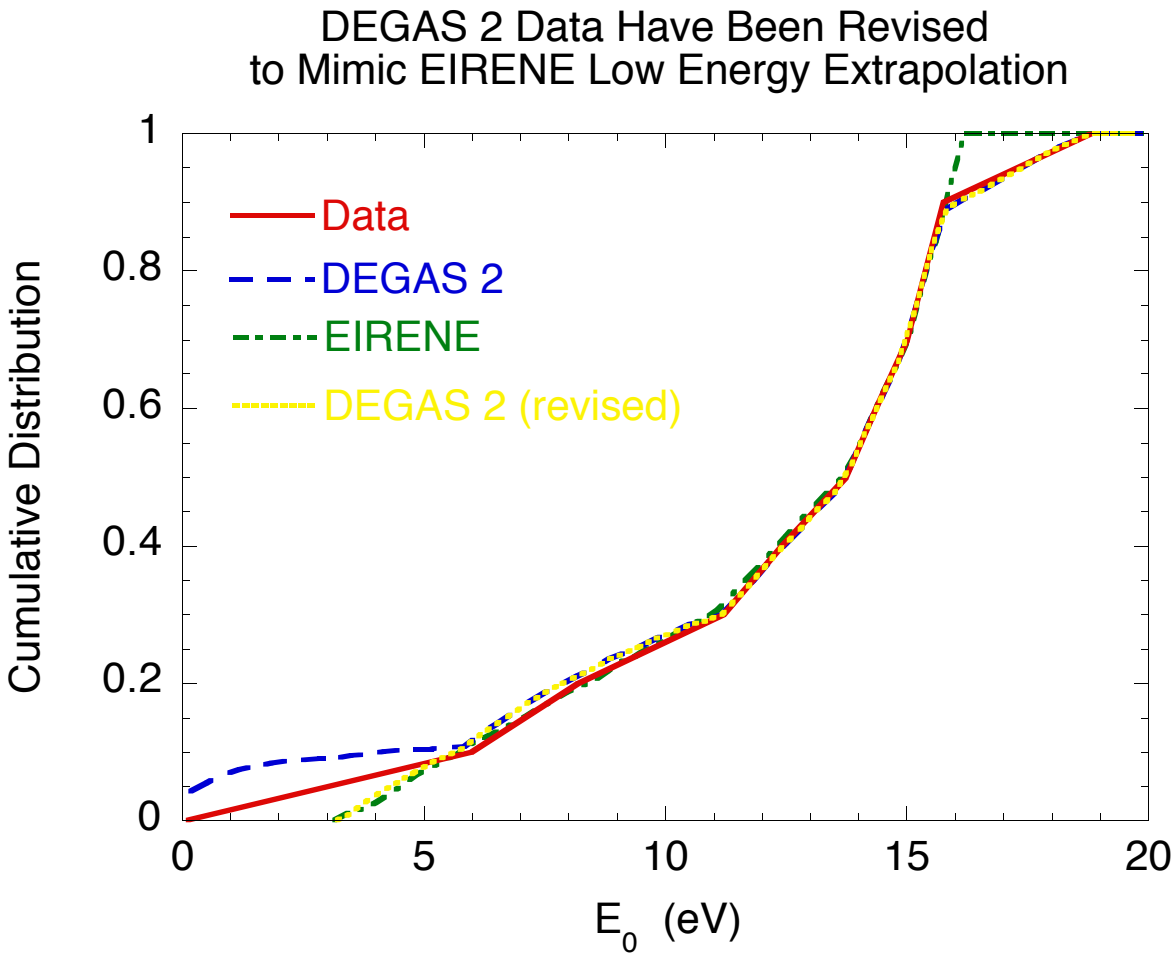


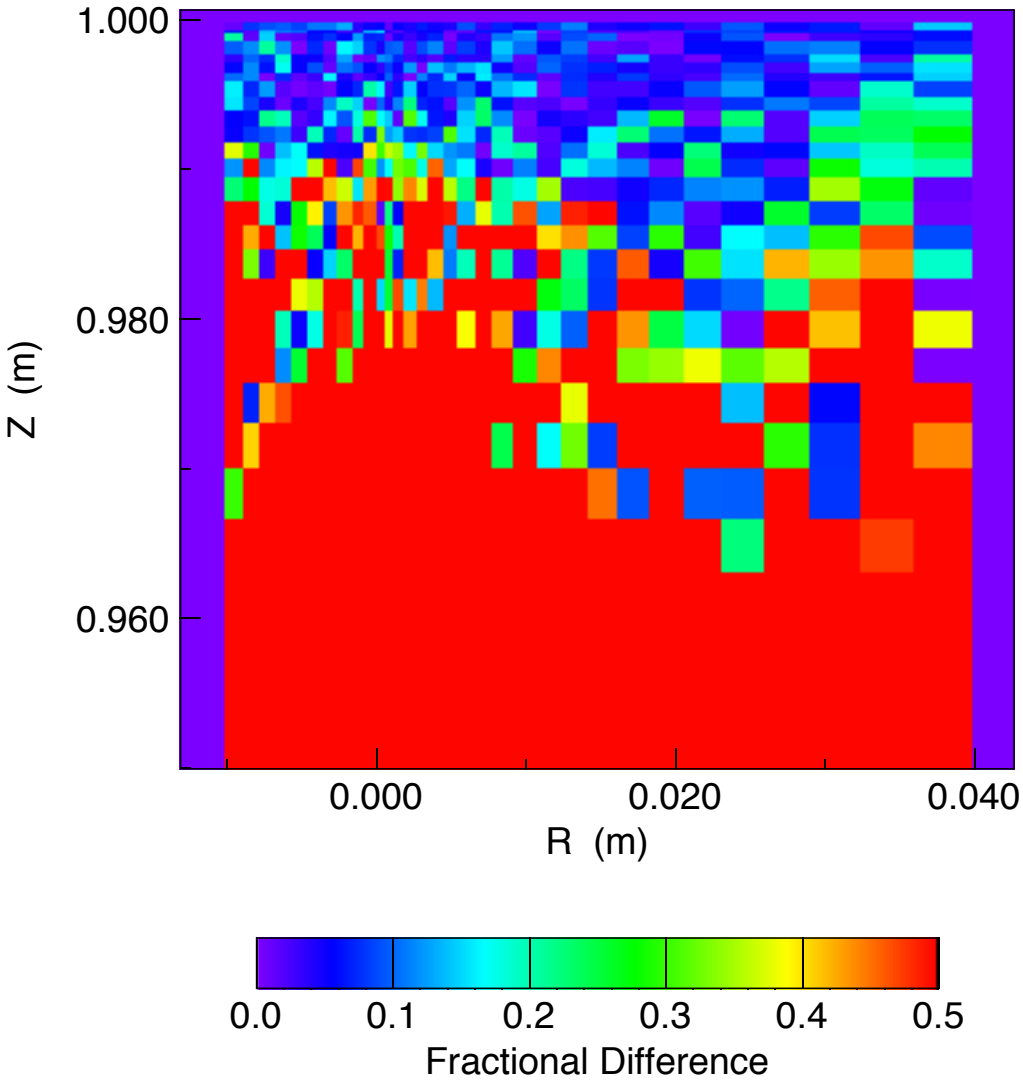
D_density vs. (row, col)



spD_density vs. (row, col)


DEGAS 2 Data Have Been Revised
to Mimic EIRENE Low Energy Extrapolation
Cumulative Distribution
1
0.8
0.6
0.4
0.2
0
0
5
10
15
20
E0 (eV)
Data
DEGAS 2
EIRENE
DEGAS 2 (revised)

Relative Std. Dev. ~7% Near Target, Increasing Rapidly Away From I



diff vs. (row, col)

EIRENE PHYSICS

- Add molecular reactions,
- Small numerical differences in low energy reflections persist,
  - $\Rightarrow$ take 5% as goal for good agreement,
  - In regions where σ smaller.
  - Other numerical differences also make doing better difficult.
- Plasma sources:
  - D^+ source rates agree within 5%,
  - Electron energy source, agreement better than 5%,
  - Momentum and ion energy sources,
    - Due to CX, error bars larger than in the above,
    - But, code results agree to within those errors.

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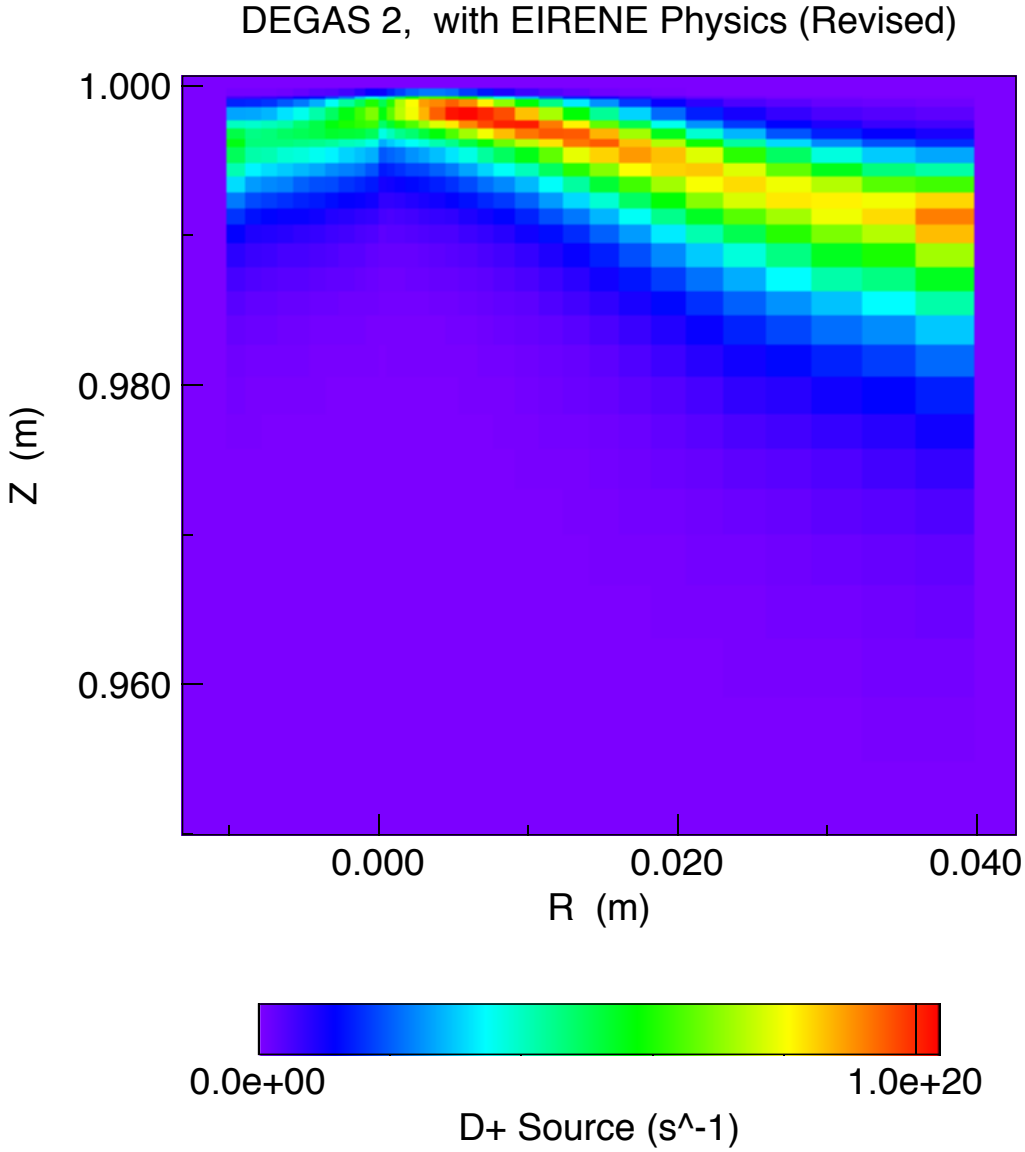
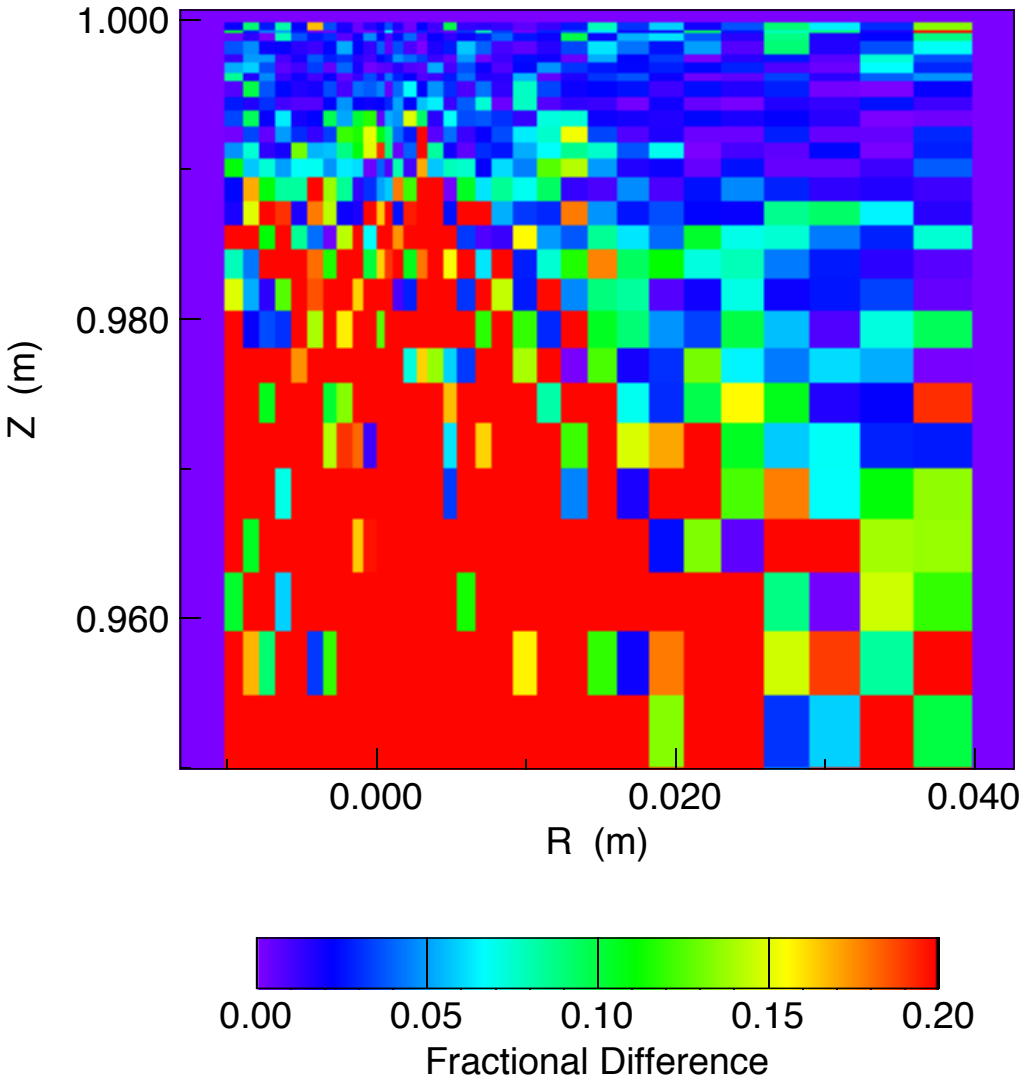
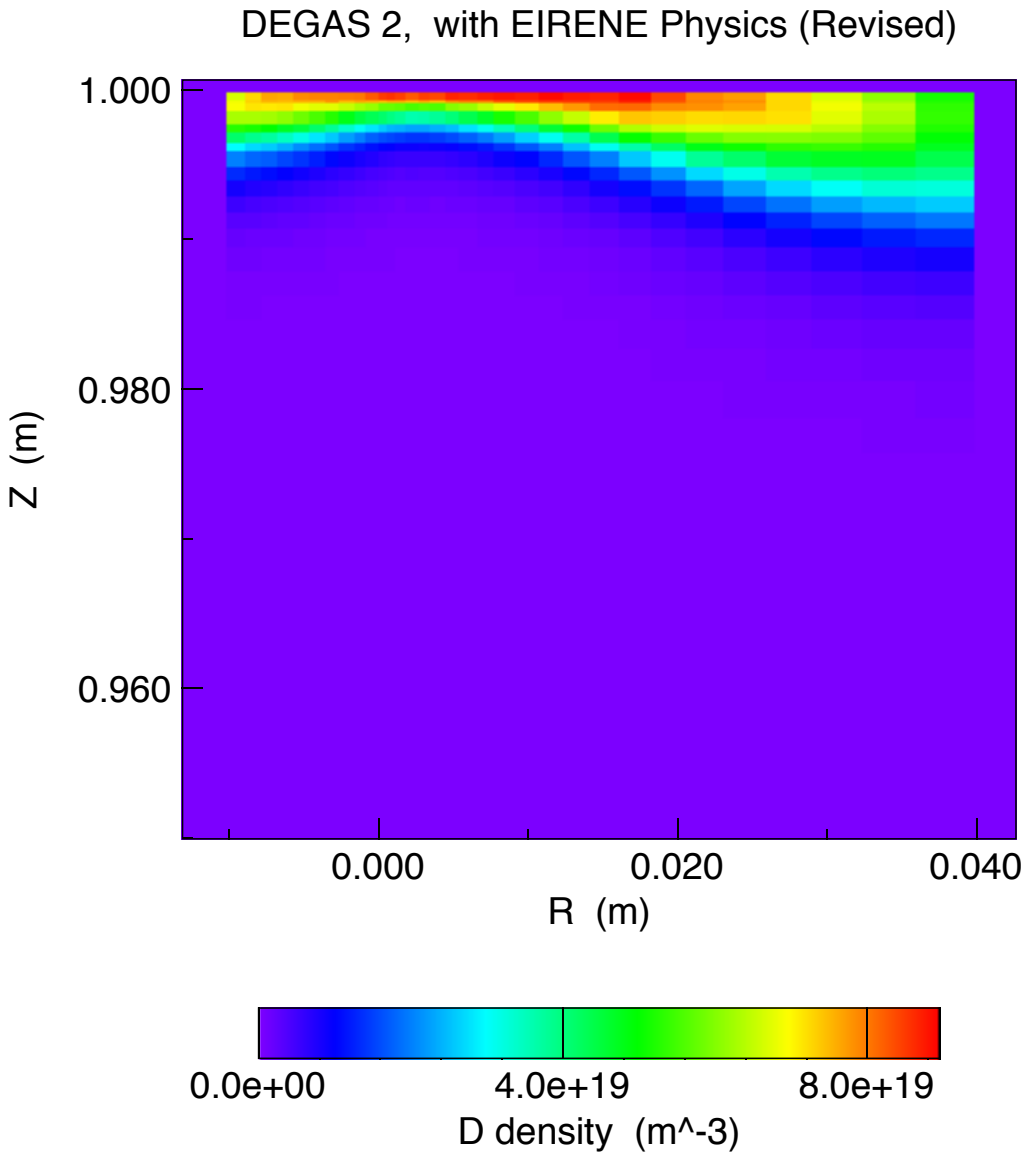


D__Ion_Source_rate vs. (row, col)

DEGAS 2 vs. EIRENE: Ion Source, with EIRENE Physics (Revised

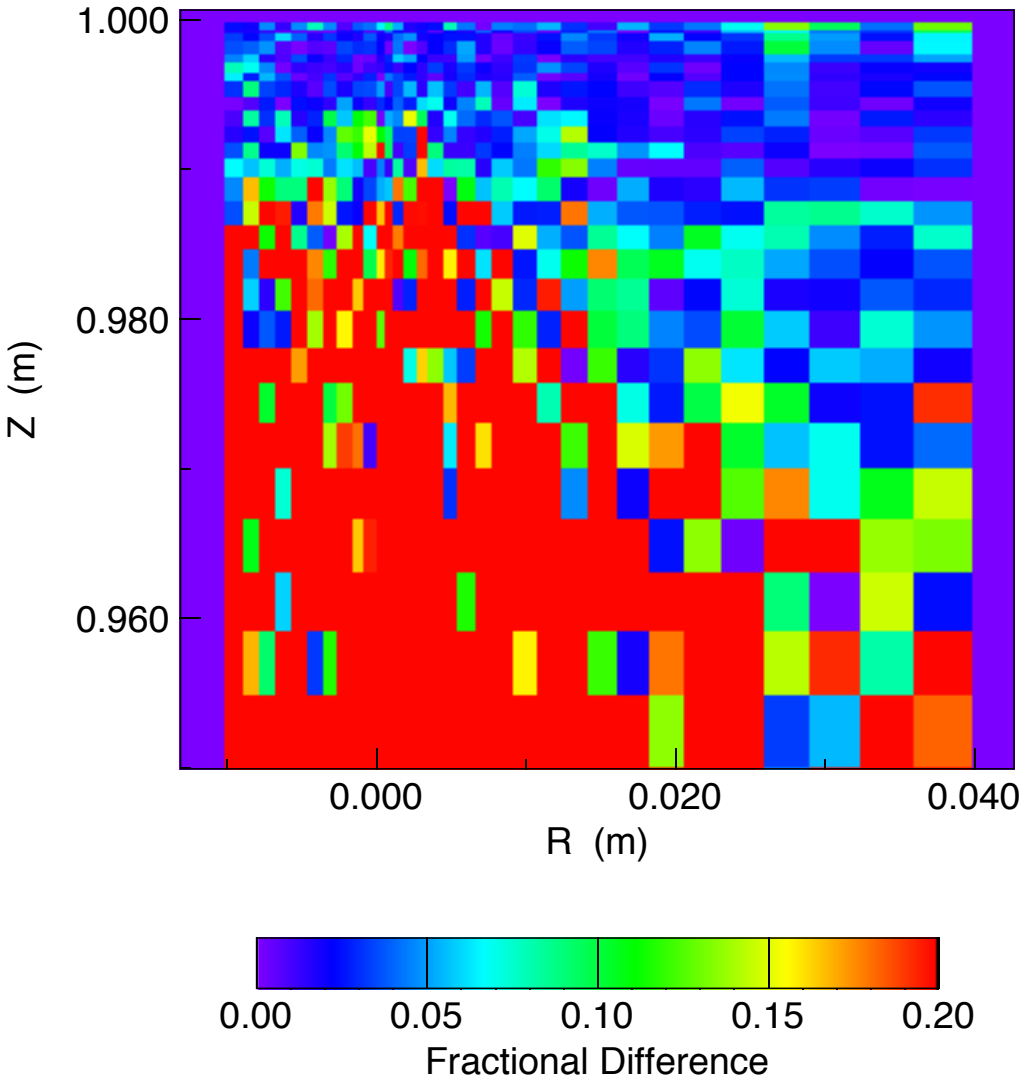


diff_sni vs. (row, col)

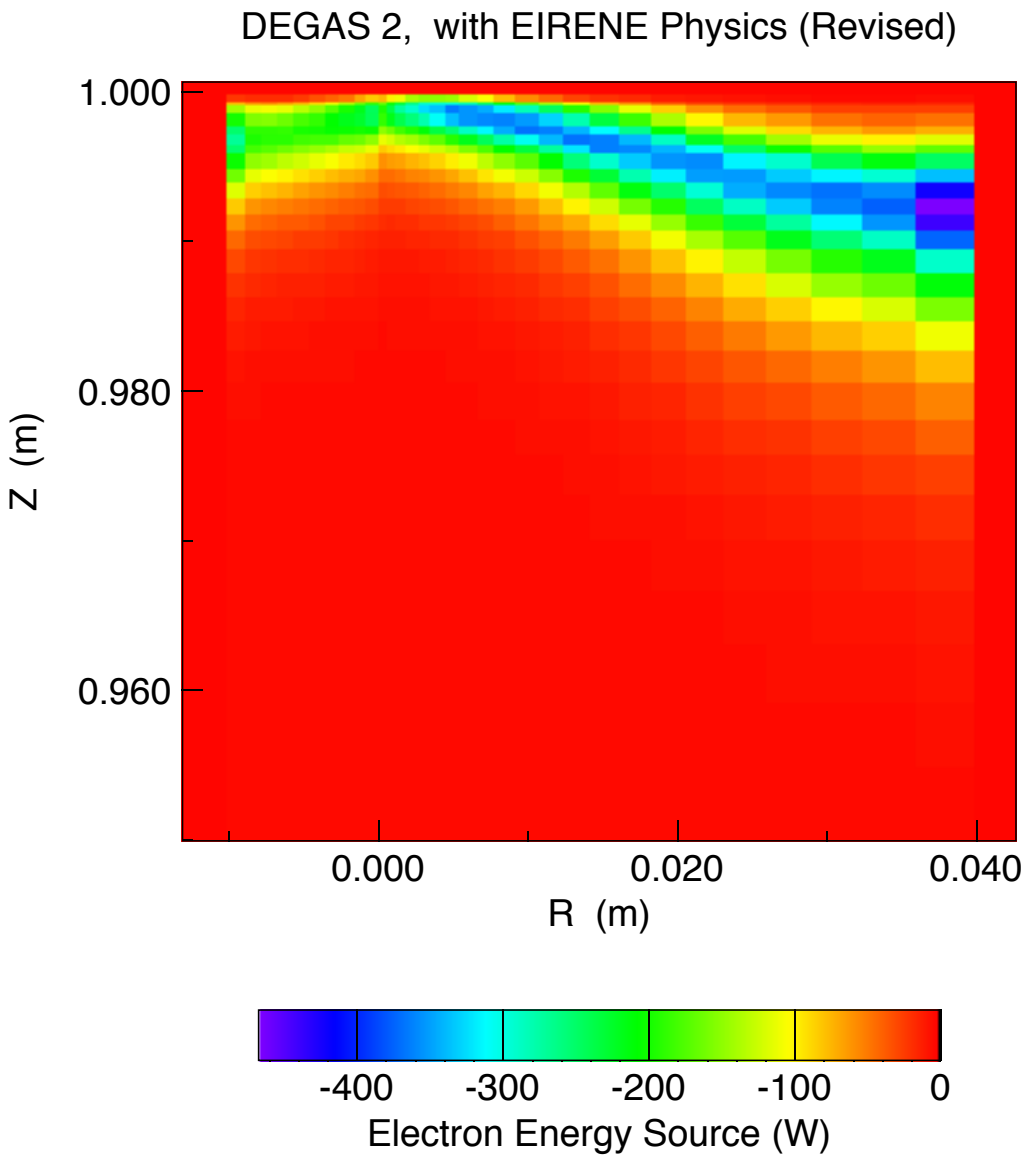


spD_density vs. (row, col)

DEGAS 2 vs. EIRENE: D Density, with EIRENE Physics (Revised

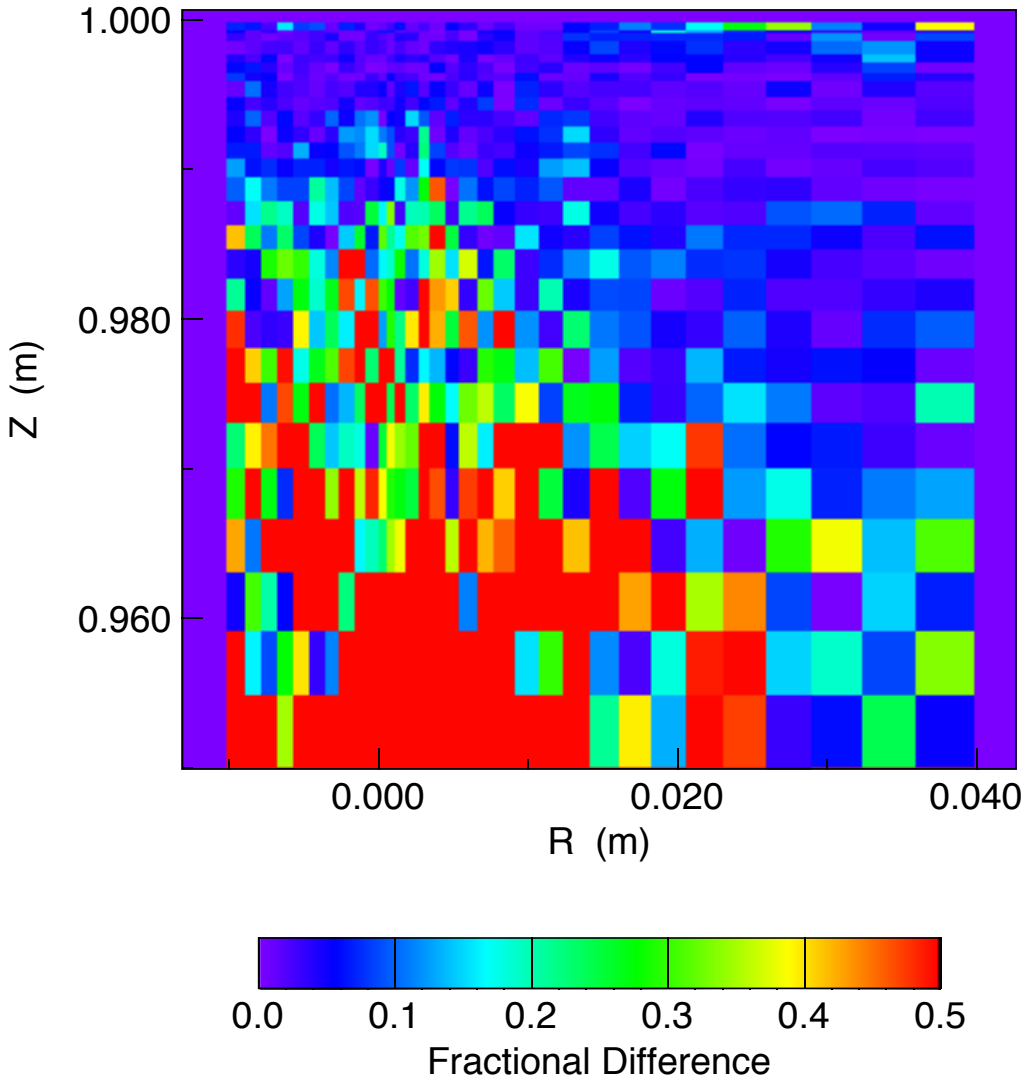


diff vs. (row, col)



e_Energy_Source_rate vs. (row, col)

DEGAS 2 vs. EIRENE: Electron Energy, with EIRENE Physics (Revised



diff_see vs. (row, col)

PERFORMANCE BENCHMARK

- Assessed, optimized single processor performance of DEGAS 2.
- Required some significant code revisions,
- Evaluated some simple algorithm changes.

1. Eliminate run-time use of string variables,
   $\sim$ 10 second reduction per 1000 flights.
2. Baseline run is above benchmark with "EIRENE physics".
   - All times are on a Sun Ultra Creator 2200,
     using F77 with "-O4" optimization.

   Baseline: 136 seconds per 1000 flights.
3. Disable charge exchange rejection,
   - Not used in this version of EIRENE,

   Disable CX rejection 119 seconds 1000 flights.
4. Reduce number of scores from 14 to 7,
   - Always track variance as well,

   Cut number of scores to 7: 95 seconds.
5. Compress scoring arrays,
   - Previously were adding $0 + 0$ *many, many* times,

   Compressed scores: 49 seconds.

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6. Removed suppressed absorption,
    - As done in EIRENE,
    - Impact on variance examined below,

    Without suppressed ionization: 15 seconds.

7. Replace track-length estimators for reactions with collision estimators,
    - Since the collision routines have to be executed anyway . . . ,
    - Again, will impact variance,

    Collision estimator: 10 seconds.

8. Follow only one H_2 product, in two atoms,
    - "Russian roulette",
    - Done this way in EIRENE and DEGAS,
    - Will impact variance,
    - Reverted to track-length estimators.

    Russian roulette on H_2: 8 seconds.

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- Figure of merit is variance times run time.
- Use region containig 83% of ion source to get estimate of variance,
- Compare variance (relative to Baseline) and run time for the above configurations:

Configuration	Seconds / 1000 Flights	σ Ratio	FOM
Baseline	49	1	49
No Ionization Suppression	15	1.9	54
Collision Estimator	10	4.3	185
H_2 Russian Roulette	8	2.3	41

- Collision estimator not a winner,
- Suppressed ionization is a wash,
- Russian roulette on molecular product looks good,
- This is default EIRENE configuration!
- Results are problem-dependent.

EIRENE performance: 12 seconds.

$\Rightarrow$ Codes now have about the same run times and give the same answers!

- With dynamic memory allocation, DEGAS 2 used 7 MB during these tests,
- EIRENE used 140 MB (geometry dimensions probably could have been set smaller).

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UPDATE

- Removing variance computations and eliminating unneeded tallies from EIRENE: EIRENE performance: 3 seconds. Will revisit later.
- Make EIRENE dimensions more appropriate for this geometry, code size reduced from 140 MB to 55 MB.

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MPI VERSION OF DEGAS 2

- DEGAS 2 designed for MPP use from beginning,
- Initially implemented PVM,
- But now have switched to MPI since it is in wider use,
- Also motivated by deployment of Princeton University's new SGI Origin 2000 machine (64 processor),
- Compare run times for a 5000 flight box run (different from above) on single processor,
- Compiler optimization on in all cases,

Digital (Alpha 500)	56 seconds
SGI (Origin 2000)	86
Sun (Ultra Creator 2200)	166
Cray (T3E)	165
Cray (C90)	435

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Multiprocessor speeds:

- 1 processor $\leftrightarrow$ CPU time (in seconds),
- Others are wall-clock time,
- Parenthetical numbers are speed-up factors relative to single processor,

No. of processors	1	10	32
SGI (Origin 2000)	86	11 (8)	4 (20)
Cray (T3E)	165	25 (6)	10 (16)

- DEGAS 2 fairly well optimized for single processor,
- MPI performance can be improved still,
- By design, MPI and single processor runs give same answer,
- Crays use F90; others, F77.
  - SGI and Sun F90 compiler have bugs,
  - Digital compiler yields very inefficient code.
- Can also explore use of shared memory on SGI Origin 2000.

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